

# NMR analog of Bell's inequalities violation test

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**Abstract.** In this paper we present an analog of the Bell's inequalities violation test for  $N$  qubits to be performed in a nuclear magnetic resonance (NMR) quantum computer. This can be used to simulate or predict results for different Bell's inequalities tests, with distinct configurations and larger number of qubits. To demonstrate our scheme, we implemented a simulation of the violation of Clauser, Horne, Shimony and Holt (CHSH) inequality using a two qubit NMR system and compared the results to those of a photon experiment. The experimental results are well described by Quantum Mechanics theory and a Local Realistic Hidden Variables model which was specially developed for NMR. That is why we refer to this experiment as a *simulation* of the Bell's inequality violation. Our result shows explicitly how both theories can be compatible to each other due the detection loophole. In the last part of this work we discuss the possibility of testing fundamental features of quantum mechanics using NMR with highly polarized spins, where a strong discrepancy between quantum mechanics and hidden variables models can be expected.

## 1. Introduction

Since the birth of Quantum Mechanics theory, interesting questions have been raised, some of them remaining not completely understood. One of the most amazing concerns the EPR paradox, brought up by Einstein, Podolsky and Rosen [1]. In that work, the authors stated that Quantum Mechanics theory is not complete since it does not contain what they called “elements of Reality”. The EPR correlations, which exists in the so-called entangled states, have no dependence on distance, which initially led to the wrong conclusion that they would violate the theory of relativity. One attempt to overcome the strange features of entangled states is to postulate the existence of some supplementary variables outside the scope of Quantum Mechanics, called “Hidden Variables” [2]. A Hidden Variables Model is supposed to reproduce all the Quantum Mechanical predictions.

However, in 1965 John Bell [3] discovered a conflict between Quantum Mechanics and the Hidden Variables theory. Mathematically, this conflict takes the form of a set of inequalities (called Bell’s inequalities), which can be violated by entangled states, but it is never violated by non-correlated quantum states or classical “objects”. Recently, there has been an increasing interest in the Bell’s inequalities subject, not only to test local realism in Quantum Mechanics in a variety of contexts, but also because of their connection to quantum communication [4, 5, 6] and quantum cryptography [7, 8]. Furthermore, Bell’s inequalities can be a useful tool to detect entanglement, which is found to be a powerful computational resource in quantum computation [9].

Violation of Bell’s inequalities has been verified in various experiments [10, 11, 12, 13, 14, 15, 16, 17, 18]. The recent development in the field of Nuclear Magnetic Resonance Quantum Information Processing (NMR-QIP) has shown that NMR is a valuable testing tool for the new ideas in quantum information science (for recent reviews see [19, 20, 21, 22]). NMR Experiments with as many as 12 qubits have been reported [23, 24]. More than fifty years of development has put NMR in an unique position to perform complex experiments, sometimes quoted as “spin choreography” [25]. Particularly fruitful has been the use of NMR-QIP to simulate quantum systems [22].

In this work, we use a NMR system to simulate a quantum optics experiment. We built a scheme to simulate the violation of Bell’s inequalities for  $N$  qubits [26, 27], and tested it in the violation of Clauser, Horne, Shimony and Holt (CHSH) inequality [28] using a two qubit NMR system. The experimental results were compared to the Quantum Mechanical theoretical predictions and also to a Local Realistic Hidden Variables model (LRHVM), built to explain the correlations observed in NMR experiments [29]. We found that both theories are consistent with our experiment and that is why we refer to the experiment a *simulation*. The consistence between both theories can be understood by the fact that NMR can detect only a small fraction of spins due to its small polarization at room temperature. A situation that resembles the so called detection loophole.

It is important to stress that the NMR qubits are nuclear spins of atoms bounded together in a single molecule, separated by few angstroms. Therefore, a NMR experiment is inherently local and cannot be used to prove nonlocal effects. Furthermore, most NMR-QIP experiments are performed at room temperature in a macroscopic liquid sample containing a large number of molecules, each of them working as an independent “quantum information processing unit”. In the NMR context, the ensemble of spins constitute a highly mixed state and their density matrix is not entangled, as demonstrated by Braunstein et al. [30]. Therefore, our work does not provide an experimental procedure to prove or disprove nonlocal effects nor reveal entanglement in NMR experiments at room temperature. However, it does provide a way to simulate tests for different Bell's inequalities. The comparison between our experiment and a true quantum optics experiment shows the faithfulness of the simulation. Besides, our scheme can be applied to a highly polarized spin ensemble [31]. In this case true entangled states can be achieved and a contradiction between hidden variables models and quantum theory could be detected.

## 2. Bell's inequalities and NMR

In this work, we refer to a generalization of the Bell's inequalities for  $N$  qubits developed in [26, 27]. It involves the measurement of a set of correlation functions, for which, each one of  $N$  observers can choose one of the  $M$  observables, whose measurements can yield only two possible values,  $s = \pm 1$ . Hence,  $M^N$  correlation functions, named  $E(n_1, \dots, n_N)$ , can be constructed, where the index  $n_i$  runs from  $n_i = 1, \dots, M$ , and denotes the settings of the  $i^{th}$  observer. For the NMR case, these observables are projections of the  $1/2$  nuclear spins along a particular direction labeled  $n_i$ . Taking into account the measurement of these observables, it is possible to build different Bell's inequalities, each of them exhibiting contradictions with LRHVM's predictions for some entangled states.

A general expression for the Bell's inequalities can be written as [32]:

$$-L \leq \sum_{n_1, \dots, n_N=1}^M C(n_1, \dots, n_N) E(n_1, \dots, n_N) \leq +L \quad (1)$$

where  $C(n_1, \dots, n_N)$  are real coefficients,  $L$  is some limit imposed by local realism and the correlations functions are given by:

$$E(n_1, \dots, n_N) = \sum_{s_1, \dots, s_N=\pm 1} \left( \prod_j^N s_j \right) P(s_1, \dots, s_N) \quad (2)$$

being  $P(s_1, \dots, s_N)$  the probability of the first observer finding the outcome  $s_1$ , the second  $s_2$  and so on. In a standard experiment, a set of  $N$  correlated particles is prepared in a pure entangled state, and their spin projection onto  $M$  different directions are measured by different observers. After a large number of runs, the observers compare

their results in order to obtain the probabilities shown in (2) and verify whether the inequality (1) was violated.

NMR experiments are described by density matrices of the kind  $\rho_{eq} \approx (\hat{I} - \beta H)/2^N$ , being  $\beta$  the Boltzmann factor and  $H$  the internal Hamiltonian of the spin system. Only the deviation of the density matrix from unity is observed. To use such a state to simulate the violation of (1) in a NMR quantum computer, the initial state is prepared from the thermal equilibrium into a highly mixed state called pseudo-pure state (PPS) [33]:

$$\rho_{pps} = \frac{(1 - \epsilon)}{2^N} \hat{I} + \epsilon |\psi\rangle\langle\psi| \quad (3)$$

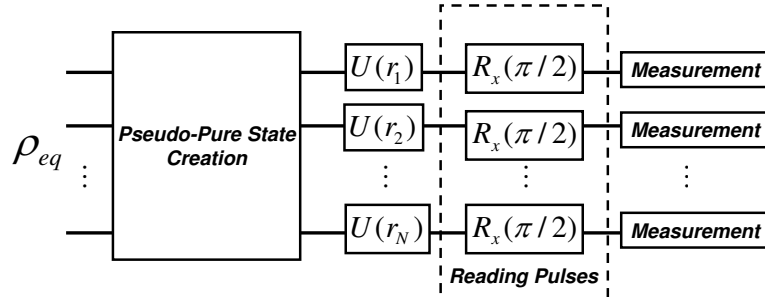
being  $\epsilon \sim 10^{-6}$ , the polarization at room temperature. It is important to remember that the last part of equation (3) represents a pure state and under an unitary transformation it behaves as such. In order to measure the spin projection  $\mathbf{r} \cdot \sigma$  onto an arbitrary direction  $\mathbf{r} = (\cos(\phi)\sin(\theta), \sin(\phi)\sin(\theta), \cos(\theta))$ , unitary transformations can be used to rotate the eigenvectors of the operator  $\mathbf{r} \cdot \sigma$  (being  $\sigma$  a vector whose components are the Pauli matrices  $\sigma_x$ ,  $\sigma_y$  and  $\sigma_z$ ) onto the computational basis. Since  $U^\dagger(\mathbf{r})\sigma_z U(\mathbf{r}) = \mathbf{r} \cdot \sigma$  for  $U(\mathbf{r}) = R_y(-\theta)R_z(-\phi)$ , by applying the appropriate  $U(\mathbf{r})$  on each qubit, we have

$$\begin{aligned} E(n_1, \dots, n_N) &= Tr(\rho_{pps} \mathbf{r}_1 \cdot \sigma \otimes \dots \otimes \mathbf{r}_N \cdot \sigma) \\ &= Tr(\rho' \sigma_z \otimes \dots \otimes \sigma_z) \end{aligned} \quad (4)$$

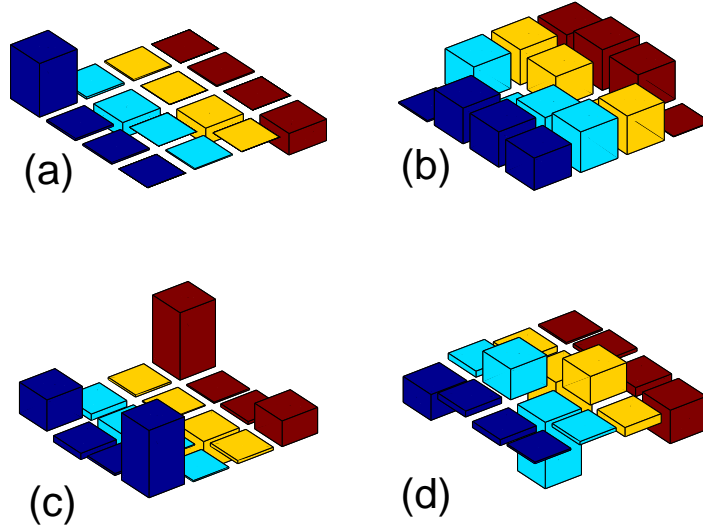
where  $\rho' = U(\mathbf{r}_1) \otimes \dots \otimes U(\mathbf{r}_N) \rho_{pps} U^\dagger(\mathbf{r}_N) \otimes \dots \otimes U^\dagger(\mathbf{r}_1)$ . The above equation tells us that the measurement of  $E(n_1, \dots, n_N)$  can be achieved by rotating each qubit by an appropriate individual rotation and then measuring them all in the computational basis. The projective measurement in the computational basis can be emulated by applying a magnetic field gradient [34], which causes the non-diagonal elements of the density matrix to vanish. The density matrix then becomes:

$$\rho' = \frac{(1 - \epsilon)}{2^N} \hat{I} + \epsilon \begin{bmatrix} P_{0\dots 0} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & P_{1\dots 1} \end{bmatrix} \quad (5)$$

The populations in the second term of (5) represent the probabilities of finding the rotated system in one of the  $2^N$  energy levels. Furthermore, they are also the probabilities  $P(s_1, \dots, s_N)$  shown in (2), which can be recovered from the NMR signal after applying reading pulses to each spin. The signal detected is the average magnetization of the sample over time, which is proportional to the difference of populations [25, 22]. The acquired signal is then Fourier transformed and normalized by a reference input state. Such a normalization allows the comparison between the experiment and theoretical results. The scheme to measure correlation functions is shown in Figure (1). The circuit must be run to each correlation function appearing in Equation (1).



n of Eq. (2).



**Figure 2.** The real part of deviation density matrices determined experimentally for the investigated pseudo-pure states (a)  $|00\rangle$ , (b)  $(|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$ , (c)  $(|00\rangle + |11\rangle)/\sqrt{2}$ , and (d)  $(|01\rangle - |10\rangle)/\sqrt{2}$ .

In order to demonstrate our scheme, we used a two-qubit NMR system, namely the nuclear spins of  $^1\text{H}$  and  $^{13}\text{C}$  in chloroform ( $\text{CHCl}_3$ ), to simulate the violation of the CHSH's inequality [28], which is a special case of (1). It involves the measurement of the quantity

$$CHSH = E(n_1, n_2) + E(n_3, n_2) + E(n_3, n_4) - E(n_1, n_4) \quad (6)$$

where  $CHSH$  is bounded by  $-2 \leq CHSH \leq +2$  for any LRHVM, whereas the limits imposed by Quantum Mechanics are given by Tsirelson's bounds  $\pm 2\sqrt{2}$  [35]. A particularly interesting situation occurs when the parameters  $n_1$ ,  $n_2$ ,  $n_3$  and  $n_4$  labels a measurement in the directions  $(0, 0, 1)$ ,  $(\sin(2\theta), 0, \cos(2\theta))$ ,  $(\sin(4\theta), 0, \cos(4\theta))$  and  $(\sin(6\theta), 0, \cos(6\theta))$ , respectively. In this case, Quantum Mechanics predicts that  $CHSH = 3\cos(2\theta) - \cos(6\theta)$  for the pure entangled state  $|\psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$  (the also called cat state), which results in a maximal violation of CHSH's inequality for  $\theta = 22.5^\circ$  and  $\theta = 67.5^\circ$ .

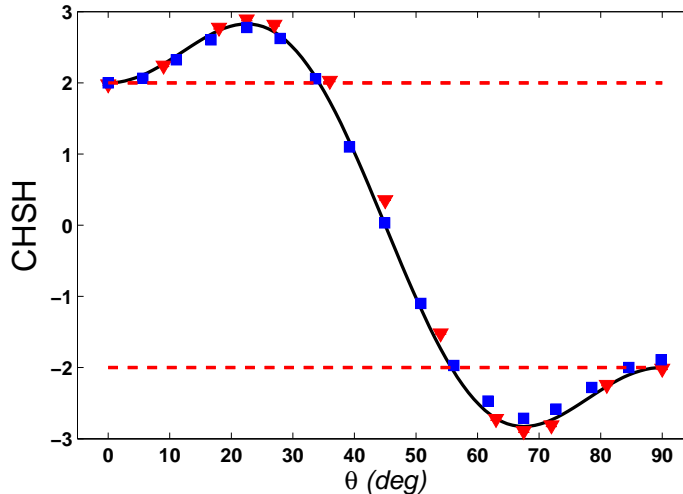
The NMR experiment was implemented in a Bruker Avance 500 MHz spectrometer in the Bruker BioSpin facility in Germany. The sample contained 99%  $^{13}\text{C}$  labeled

chloroform dissolved in deuterated dichlorometane ( $CD_2Cl_2$ ), and the concentration was close to 200 mg of  $CHCl_3$  per 1 ml of  $CD_2Cl_2$ . Pseudo-pure states were prepared by the spatial average technique, for which pulse sequences can be found in [34]. Density matrices were reconstructed by using quantum state tomography [36, 37]. The real parts of the experimental deviation density matrices  $\rho_{exp}$  of the investigated states are shown on Figure (2). The deviation  $\delta = \frac{\|\rho_{exp} - \rho_{id}\|_2}{\|\rho_{id}\|_2}$  from the ideal pseudo-pure density matrices  $\rho_{id}$  are below 10% in all cases, and the imaginary parts were found to be negligible compared to the real part. The errors are mainly due to radio frequency field inhomogeneity and small pulse imperfections. The decoherence is not a important source of errors since the time required of entire experiment ( $\sim 15$  ms) is much smaller then the estimated decoherence time,  $T1 \sim 5$  s ( $T1 \sim 15$  s) and  $T2 \sim 200$  ms ( $T2 \sim 300$  ms) for hydrogen (Carbon).

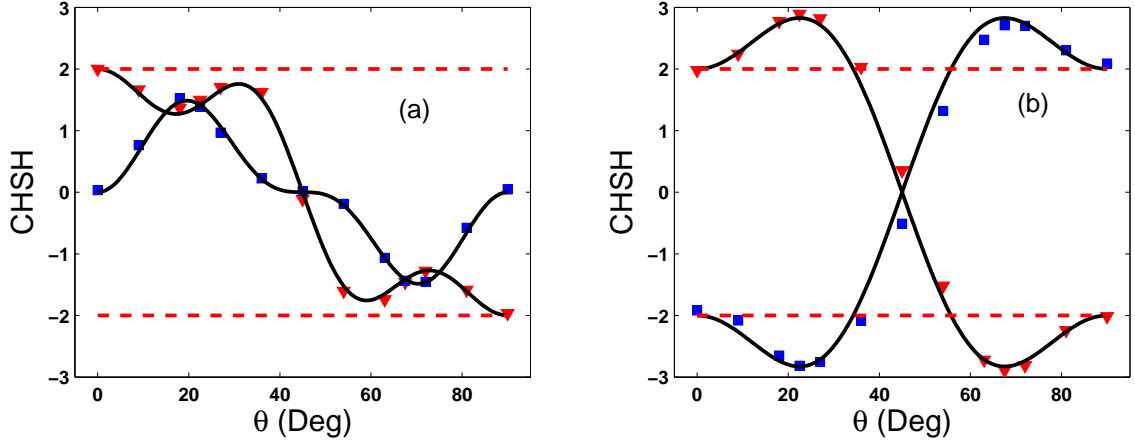
The experimental results for the cat state can be seen in Figure (3), where the  $CHSH$  quantity is shown as functions of the angle  $\theta$ . The experimental results are also compared to the Quantum Mechanical predictions for a pure cat state and with a photon experiment of CHSH's inequality test extracted from Ref. [10]. As it can be seen, our experiment is in good agreement with both, the Quantum Mechanics theory and the photons experiment.

### 3. Comparison with a hidden variable model

The density matrix (3) can be decomposed in an ensemble in which the fraction  $\epsilon$  of the system is in a pure state  $|\psi\rangle$  while the rest are in a completely mixed state, however it is not the unique decomposition allowed. Braunstein et al. [30] has demonstrated that any matrix of the form (3) can be decomposed in a separable ensemble whenever  $\epsilon \leq 1/(1+2^{N-1})$ . This remarkable result shows that although the pseudo-pure state (3)



**Figure 3.** Experimental results for the cat state.  $\blacktriangledown$  NMR experiment,  $\blacksquare$  Photon experiment taken from [10]. The solid line is the Quantum Mechanical predictions.



**Figure 4.** Experimental results of the  $CHSH$  quantity as function of the angle  $\theta$ . (a)  $\blacktriangledown$   $|00\rangle$ ,  $\blacksquare$   $(|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$ . (b)  $\blacktriangledown$   $(|00\rangle + |11\rangle)/\sqrt{2}$ ,  $\blacksquare$   $(|01\rangle - |10\rangle)/\sqrt{2}$ . The continuous lines are the predictions of the LRHVM described in [29]. The NMR data showed here are the same as in figure (3)

can be used to implement any quantum computation, it is classical correlated and may have a local realistic description which was later given explicitly in [29].

In this section, we have compared our results to an explicit LRHVM [29]. This model is constructed to predict the Quantum Mechanical expectation values of any bulk-ensemble NMR experiments that access only separable states. The most general type of transformation of quantum states (unitary or not) can be described via operator sum representation  $\rho \rightarrow \sum_k E_k \rho E_k^\dagger$  ( $\sum_k E_k^\dagger E_k = \hat{I}$ ) [9]. With this formalism it is possible to simulate every step of our experiment, taking the elements of operation  $E_k$  as model's parameter. Starting from the NMR equilibrium density matrix  $\rho_{eq}$ , we simulated every spectra and analyzed them in the same way as we did for experimental data. The relaxation effects were taken into account using the elements of operation described in [38].

In Figure (4a), it is shown the experimental results for the states  $|00\rangle$  and  $(|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$  compared with predictions of the LRHVM described in [29]. As it can be seen, there is no violation of the CHSH's inequality for these two states, as predicted by both Quantum Mechanics theory and LRHVM, since they are separable states.

The experimental results for the states  $(|00\rangle + |11\rangle)/\sqrt{2}$  and  $(|01\rangle - |10\rangle)/\sqrt{2}$  are shown in Figure (4b). Here we found a violation of the CHSH's inequality in good agreement with Quantum Mechanics theory. Additionally, our results are also in good agreement with the LRHVM. The fact that our experimental data is compatible to both theories may appear puzzling. However, it can be understood, noting that NMR is only sensible to the deviation part of (3), that behaves like a "pure entangled state" although the total ensemble is classically correlated as demonstrated in [30, 29].

This situation resembles the detection loophole, usually discussed in the context



of optics. Generally in experiments testing Bell's inequalities  $\ddagger$ , imperfections on the experimental apparatus lead to the fact that only a small sub ensemble of the total number of produced entangled particles is actually detected. The question to be asked is whether the measured events is a faithful representation of the whole system. In principle, the detected sub ensemble could contain a distribution of hidden variables different from the total ensemble. Thus it is possible for the detected sub ensemble to violate the Bell's inequalities, even if the total ensemble do not, one can state that the sub ensemble "simulates" the violation of Bell's inequalities. This problem, first noted in [39], is called the detection loophole. Generally, to overcome the problem, it is invoked the fair sampling hypothesis, that state that the detected sub ensemble indeed represents the whole system.

In the case of NMR experiments, we cannot invoke this hypothesis, since the non-detected spins are known to be in highly mixed state and not in the desired entangled state. Furthermore, NMR-QIP has a known LRHVM which is in well agreement with experimental observation, as shown in (4b). Thus our experiment is indeed a simulation.

#### 4. Conclusion

In summary, we have successfully simulated a violation of a Bell's inequality test using classical means. The faithfulness of our simulation was tested by comparing our results with those of a photon experiment. We also show that we can produce the exact same set of data by using a LRHVM and Quantum Mechanics. This result can be viewed as a experimental demonstration on how both theories can be compatible due to the detection loophole. We must emphasize that such a LRHVM is valid only for NMR experiment, and not to photon one, although both curves are coincident. Besides, our protocol can be used to simulate or predict results for different Bell's inequalities tests, with distinct configurations and larger number of qubits.

It is important to mention that the same experiment carried out in a highly polarized spin ensemble would not present the same features. Recently, an almost pure NMR quantum entangled state was achieved with polarization  $\epsilon = 0.916 \pm 0.019$  [31]. The reported entanglement of formation of such state was  $0.822 \pm 0.039$ , in this situation a true violation of Bell's inequalities is expected. Particularly interesting for NMR are those inequalities which do not require entanglement [40] §, such as the temporal Bell's inequalities [41], which recent proposals based on weak measurements [42, 43] could be adapted to NMR systems, and those inequalities that do not require a space-like separation between the entangled particles, such as recently done in [11]. These inequalities are designed for the purpose to test realism.

In Figure (5), we show a computer simulation of the violation of inequality found

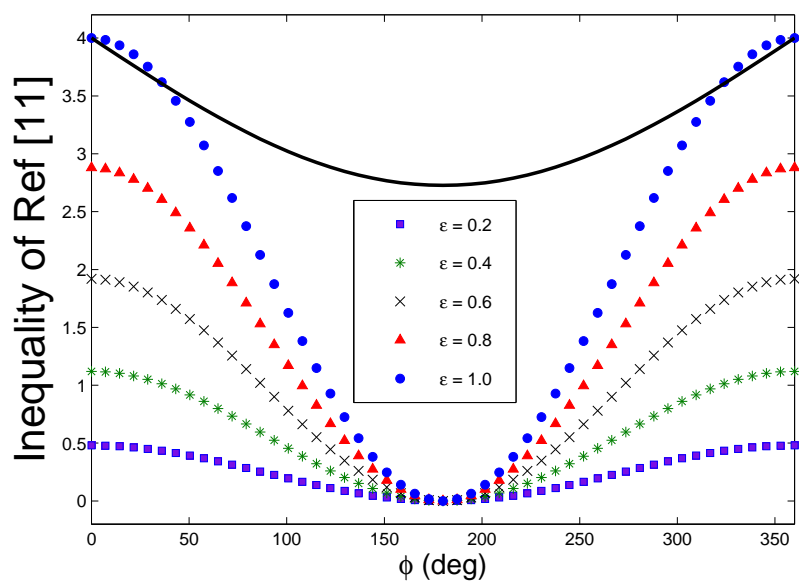
$\ddagger$  Up to now there is only one experiment [12] reporting violation of Bell's inequality without the detection loophole.

§ Note that even in this case the polarization must be enhanced because the LRHVM described in [29] also rules out the violation of such inequalities for  $\epsilon \leq 1/(1 + 2^{N-1})$ .



in [11]. We simulated the scheme described in this paper using NMR density matrix (3) for various values of spins polarization. The solid line represent the limit imposed by the realism, the region above the limit may not have a realistic description.

We are currently seeking ways to implement these test on a NMR system. Besides the ability to simulate quantum systems. We believe that NMR quantum computation could also be used to perform real tests of quantum mechanics fundamentals. This subject is less explored with NMR, however the ability to generate highly spin polarized ensemble allied to the high degree of control, could put NMR in a unique position in quantum information science.



**Figure 5.** Computer simulation of the violation of the inequality proposed in [11] for various values of the spin polarization  $\epsilon$ . The solid line represents the limit imposed by hidden variables, the points above the solid line may not have a realistic description.

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